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Abstract

Full Text

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ON THE QUANTUM THEORY OF ANISOTROPIC FERROMAGNETISM

(Presented by Academician N. N. Bogolyubov, 16 VI 1965)

In this work the results of papers (1, 2) (in which Green's thermodynamic-function method was applied to an anisotropic ferromagnet) are obtained by the method of linearization of the equations of motion, developed in (3, 4) for the isotropic case.

The system consists of N spins of length S , located at the sites of a crystal lattice, and is described by the Hamiltonian

$$H = -\mu\mathcal{H}^\alpha \sum_f S_f^\alpha - \frac{1}{2} \sum_{\substack{f,g \\ f \neq g}} P_{fg}^{\alpha\chi} S_f^\alpha S_g^\chi, \quad (1)$$

where μS is the magnetic moment of one ion, \mathcal{H}^α is a component of the external magnetic field; S_f^α is a component of the spin operator at the site f ; $P_{fg}^{\alpha\chi}$ are the components of the tensor of exchange interaction of the spins S_f^α, S_g^χ at the sites f and g ; $P_{fg}^{\alpha\chi} = P_{gf}^{\chi\alpha}$. We assume that there is a center of symmetry in the crystal. The spin operators satisfy the known commutation relations

$$[S_f^\alpha, S_g^\chi] = i\delta_{fg}\varepsilon_{\alpha\chi\tau}S_f^\tau. \quad (2)$$

The magnetization vector at the site f is defined as $\vec{\sigma}_f = \langle \mathbf{S}_f \rangle$, where $\langle \dots \rangle$ denotes averaging over the canonical ensemble with temperature $T = 1/k\beta$. For one domain (which we shall consider), $\vec{\sigma}_f$ does not depend on the lattice site: $\vec{\sigma}_f = \vec{\sigma}$. We introduce (5) a new orthonormal coordinate system, whose unit vectors we denote by $\mathbf{a}, \mathbf{b}, \tilde{\gamma}$. By definition, $\tilde{\gamma} = \vec{\sigma}/\sigma$, where σ is the length of the vector $\vec{\sigma}$. In the new coordinate system the Hamiltonian has the same form as the original one, but the quantities entering it (we denote them by primes) are expressed as follows: $\mathcal{H}'^1 = \tilde{\mathcal{H}}\mathbf{a}$, $S_f'^1 = \mathbf{S}_f\mathbf{a}$, $P_{fg}'^{12} = P_{fg}^{\alpha\chi}a^\alpha b^\chi$, etc. The further calculations will be carried out in the variables $S_f'^+, S_f'^-, S_f'^0$, defined as follows:

$$S_f'^0 = S_f'^3, \quad S_f'^\pm = S_f'^1 \pm S_f'^2. \quad (3)$$

In the new coordinate system

$$\langle S_f^\pm \rangle = 0, \quad \langle S_f^0 \rangle = \sigma.$$

The Heisenberg equations of motion for the variables (3) have the form

$$\begin{aligned} \frac{dS_f^\Gamma(t)}{dt} &= -i\Gamma\mu\mathcal{H}'^0 S_f^\Gamma(t) + i\Gamma\mu\mathcal{H}'^\Gamma S_f^0(t) + \\ &+ \frac{i}{2}\Gamma \sum_{g \neq f} P_{fg}^{\bar{\Gamma}\Lambda} S_f^0(t) S_g^\Lambda(t) + i\Gamma \sum_{f \neq g} P_{fg}^{\Gamma 0} S_f^0(t) S_g^0(t) - \\ &- \frac{i}{2}\Gamma \sum_{g \neq f} P_{fg}^{\prime 0 \bar{\Lambda}} S_f^\Gamma(t) S_g^\Lambda(t) - i\Gamma \sum_{g \neq f} P_{fg}^{\prime 0 0} S_f^\Gamma(t) S_g^0(t), \end{aligned} \quad (4)$$

$$\frac{dS_f^0(t)}{dt} = -\frac{i\mu}{2} \sum_{\Lambda} \Lambda \mathcal{H}'^{\bar{\Lambda}} S_f^\Lambda(t) + \frac{i}{4} \sum_{\substack{g \neq f \\ \Lambda, \Omega}} P_{fg}^{\bar{\Lambda}\bar{\Omega}} S_f^\Lambda(t) S_g^\Omega(t) + \frac{i}{2} \sum_{\substack{g \neq f \\ \Lambda}} \Lambda P_{fg}^{\bar{\Lambda} 0} S_f^\Lambda(t) S_g^0(t), \quad (5)$$

where $\Omega, \Lambda, \Gamma = \pm$, $\bar{\Omega} = -\Omega$, $\mathcal{H}'^0 = \mathcal{H}'^3$, $\mathcal{H}'^\Lambda = \mathcal{H}'^1 - i\Lambda\mathcal{H}'^2$, $P_{fg}^{\prime 0 0} = P_{fg}^{\prime 3 3}$, $P_{fg}^{\bar{\Lambda} 0} = P_{fg}^{\prime 1 3} - i\Lambda P_{fg}^{\prime 2 3}$, $P_{fg}^{\bar{\Lambda}\bar{\Omega}} = P_{fg}^{\prime 1 1} - \Lambda\Omega P_{fg}^{\prime 2 2} - i\Lambda P_{fg}^{\prime 2 1} - i\Omega P_{fg}^{\prime 1 2}$.

The linearization is as follows. We substitute into the equations of motion $S_f^0 = S^0 = \sigma$, and then retain on the right-hand sides of equations (4), (5) only terms linear in S_f^Λ . In this way we obtain the linearized approximate equations of motion

$$\frac{dS_f^\Gamma}{dt} = i\sigma\Gamma \left[M'^\Gamma - i\Gamma M'^0 S_f^\Gamma + \frac{i\sigma}{2}\Gamma \sum_{f \neq g} P_{fg}^{\bar{\Gamma}\Lambda} S_g^\Lambda \right], \quad (6)$$

$$\frac{dS_f^0}{dt} = \frac{i}{2} \sum_{\Lambda} \Lambda M'^{\bar{\Lambda}} S_f^\Lambda = 0, \quad (7)$$

where

$$M'^\Gamma = \mu\mathcal{H}'^\Gamma + \sigma P_0^{\Gamma 0}, \quad M'^0 = \mu\mathcal{H}'^0 + \sigma P_0^{\prime 0 0}. \quad (8)$$

It follows from (7) that the vector \mathbf{M}' is parallel to the vector $\vec{\sigma}$:

$$\mathbf{M}' = \lambda \vec{\sigma} \quad \text{or} \quad \mu\mathcal{H}'^\alpha + P_0^{\alpha\alpha} \sigma^\alpha = \lambda \sigma^\alpha.$$

This equation determines the direction of σ . To obtain an equation for the length σ , we pass to the reciprocal lattice. Equations (6) take the form

$$dS_J^+ / dt = -ip_J S_J^+ - ir_J S_J^-, \quad dS_J^- / dt = ir_J^* S_J^+ + ip_J S_J^-, \quad (9)$$

where $p_J = M'^0 - \frac{\sigma}{2} P_J'^{+-} = p_J^*$ (the reality of p_J follows from the fact that the system has a center of symmetry); $r_J = -\frac{i}{2} \sigma P_J'^{++}$.

The solutions of these equations are

$$S_J^\Gamma(t) = \varphi_J^\Gamma(t) S_J^\Gamma(0) + \chi_J^\Gamma(t) S_J^{\bar{\Gamma}}(0), \quad (10)$$

where

$$\varphi_J^+(t) = \cos(c_{Jt}) - \frac{ip_J}{c_J} \sin(c_{Jt}) = \varphi_J^{-*}(t),$$

$$\chi_J^+(t) = -\frac{ir_J}{c_J} \sin(c_{Jt}) = \chi_J^{-*}(t),$$

$$c_J = p_J^2 - r_{Jr} J^*.$$

Using the obvious relations

$$\text{Tr}(e^{-\beta H} [S_J^\Gamma, Y]) = \text{Tr}(Y [e^{-\beta H}, S_J^\Gamma])$$

(Y is for the time being an arbitrary operator),

$$S_J^\Gamma(t) = e^{iHt} S_J^\Gamma(0) e^{-iHt},$$

$$[e^{-\beta H}, S_J^\Gamma(0)] = (\varphi_J^\Gamma(i\beta) - 1) S_J^\Gamma(0) e^{-\beta H} + \chi_J^\Gamma(i\beta) S_J^{\bar{\Gamma}}(0) e^{-\beta H},$$

we obtain the equations

$$\langle [S_J^\Gamma, Y] \rangle = (\varphi_J^\Gamma(i\beta) - 1) \langle Y S_J^\Gamma \rangle + \chi_J^\Gamma(i\beta) \langle Y S_J^{\bar{\Gamma}} \rangle,$$

from which we calculate the averages

$$\langle Y S_J'^+ \rangle = Q_J \langle [S_J'^+, Y] \rangle + R_J \langle [S_J'^-, Y] \rangle,$$

$$\langle Y S_J^- \rangle = U_J \langle [S_J^+, Y] \rangle + V_J \langle [S_J^-, Y] \rangle, \quad (11)$$

where

$$Q_J = (\varphi_J^-(i\beta) - 1)' / D_J, \quad R_J = -\chi_J^+(i\beta) / D_J,$$

$$U_J = -\chi_J^-(i\beta) / D_J, \quad V_J = (\varphi_J^+(i\beta) - 1) / D_J,$$

$$D_J = (\varphi_J^+(i\beta)' - 1)(\varphi_J^-(i\beta) - 1) - \chi_J^+(i\beta)\chi_J^-(i\beta).$$

Suppose that Y depends only on one site of the direct lattice ($Y = Y_f$). Then $[S_J^T, Y_f] = e^{ifJ} [S_f^T, Y_f]$. Multiplying equations (11) by $\frac{1}{N} e^{-ifJ}$ and summing over J , we obtain

$$\langle Y_f S_f^+ \rangle = Q v^+ + R v^-, \quad \langle Y_f S_f^- \rangle = U v^+ + V v^-, \quad (12)$$

where

$$Q = \frac{1}{N} \sum_J Q_J, \quad U = \frac{1}{N} \sum_J U_J, \quad v^+ = \langle [S_f^+, Y_f] \rangle,$$

$$R = \frac{1}{N} \sum_J R_J, \quad V = \frac{1}{N} \sum_J V_J, \quad v^- = \langle [S_f^-, Y_f] \rangle.$$

If one substitutes $Y_f = (S_f^0)^n S_f'^-$, then equations (12) take the form

$$\begin{aligned} & (1 + Q) \langle (S^0)^{n+2} \rangle + (1 + Q) \langle (S^0)^{n+1} \rangle - (1 + Q) S(S+1) \langle (S^0)^n \rangle - \\ & - Q \langle (S^0 - 1)^n (S^0)^2 \rangle + Q \langle (S^0 - 1)^n S^0 \rangle + Q S(S+1) \langle (S^0 - 1)^n \rangle + \\ & + R \langle (S^0 + 1)^n (S'^-)^2 \rangle - R \langle (S^0)^n (S'^-)^2 \rangle = 0, \\ & U \langle (S^0)^{n+2} \rangle + U \langle (S^0)^{n+1} \rangle - U S(S+1) \langle (S^0)^n \rangle - \\ & - U \langle (S^0 - 1)^n (S^0)^2 \rangle + U \langle (S^0 - 1)^n S^0 \rangle + U S(S+1) \langle (S^0 - 1)^n \rangle + \end{aligned} \quad (13)$$

$$+V\langle(S'^0 + 1)^n(S'^-)^2\rangle - (1 + V)\langle(S'^0)^n(S'^-)^2\rangle = 0.$$

Adding to equations (13) the well-known Cayley-Hamilton equation

$$\left(\prod_{k=-S}^S (S^0 - k) = 0 \right)$$

and setting the exponent n equal to $0, 1, \dots, 2S - 1$, we obtain a closed system of linear equations for the averages

$$\langle(S'^-)^2\rangle, \langle S'^0(S'^-)^2\rangle, \dots, \langle(S'^0)^{2S-1}(S'^-)^2\rangle, \langle S'^0\rangle, \dots, \langle(S'^0)^{2S}\rangle.$$

From this we calculate $\sigma = \langle S'^0 \rangle$ as a function of the quantities Q, R, U, V , which, in turn, depend on σ . Thus, σ satisfies one complicated transcendental equation.

For example, for $S = 1$, $n = 0, 1$,

$$(S^0)^3 - S^0 = 0,$$

$$\langle(S^0)^2\rangle + (1 + 2Q)\langle S^0\rangle - 2 = 0, \quad 2U\langle S^0\rangle - \langle(S^-)^2\rangle = 0,$$

$$\langle(S^0)^3\rangle + (1 + 3Q)\langle(S^0)^2\rangle - (Q + 2)\langle S^0\rangle + R\langle(S^-)^2\rangle - 2Q = 0,$$

$$3U\langle(S^0)^2\rangle - U\langle S^0\rangle - \langle S^0(S^-)^2\rangle + V\langle(S^-)^2\rangle - 2U = 0.$$

Hence

$$\sigma = \frac{2Q + 1}{3Q^2 + 3Q - UR + 1}.$$

In an analogous way, for $S = \frac{3}{2}$,

$$\sigma = \frac{3(10Q^2 + 10Q - 5UR + 3)}{24Q^3 + 36Q^2 + 23Q - 8UR - 20URQ + 4UVR + 6}.$$

For the simple example of a uniaxial anisotropic ferromagnet, for which

$$P_{fg}^{\alpha\beta} = \delta_{\alpha\beta}P_{fg}^\alpha, \quad p_{fg}^1 = p_{fg}^2 = P_{fg}, \quad p_{fg}^3 = P_{fg} + \Delta_{fg},$$

the problem is solved uniquely for a definite sign of Δ_{fg} and a definite choice of the magnitude and direction of the external magnetic field. The uniqueness is directly connected with the requirement that the coefficients of the equations solved in the problem be finite. These coefficients diverge if c_J tends to zero. It turns out that there always exists one and only one solution that does not lead to zero c_J . These solutions coincide with the results of works ^(1,2).

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